High performance electronic structure engineering[1] MARCO GOV-ONI, GIULIA GALLI, Institute for Molecular Engineering, The University of Chicago; Materials Science Division, Argonne National Laboratory — We discuss the efficiency of a recently proposed method for the calculation of energy levels in condensed and finite systems with density functional theory and many-body perturbation theory at the GW level. We present applications of this technique to the calculation of electronic properties of systems with thousands of electrons, including semiconductor nanoparticles, solid/liquid interfaces and defective materials. In addition we discuss the parallel performance and scalability on high performance architectures of a newly developed code [1], implementing the method.

[1] M. Govoni and G. Galli, Large scale GW calculations, submitted.

Marco Govoni
Institute for Molecular Engineering, The University of Chicago;
Materials Science Division, Argonne National Laboratory